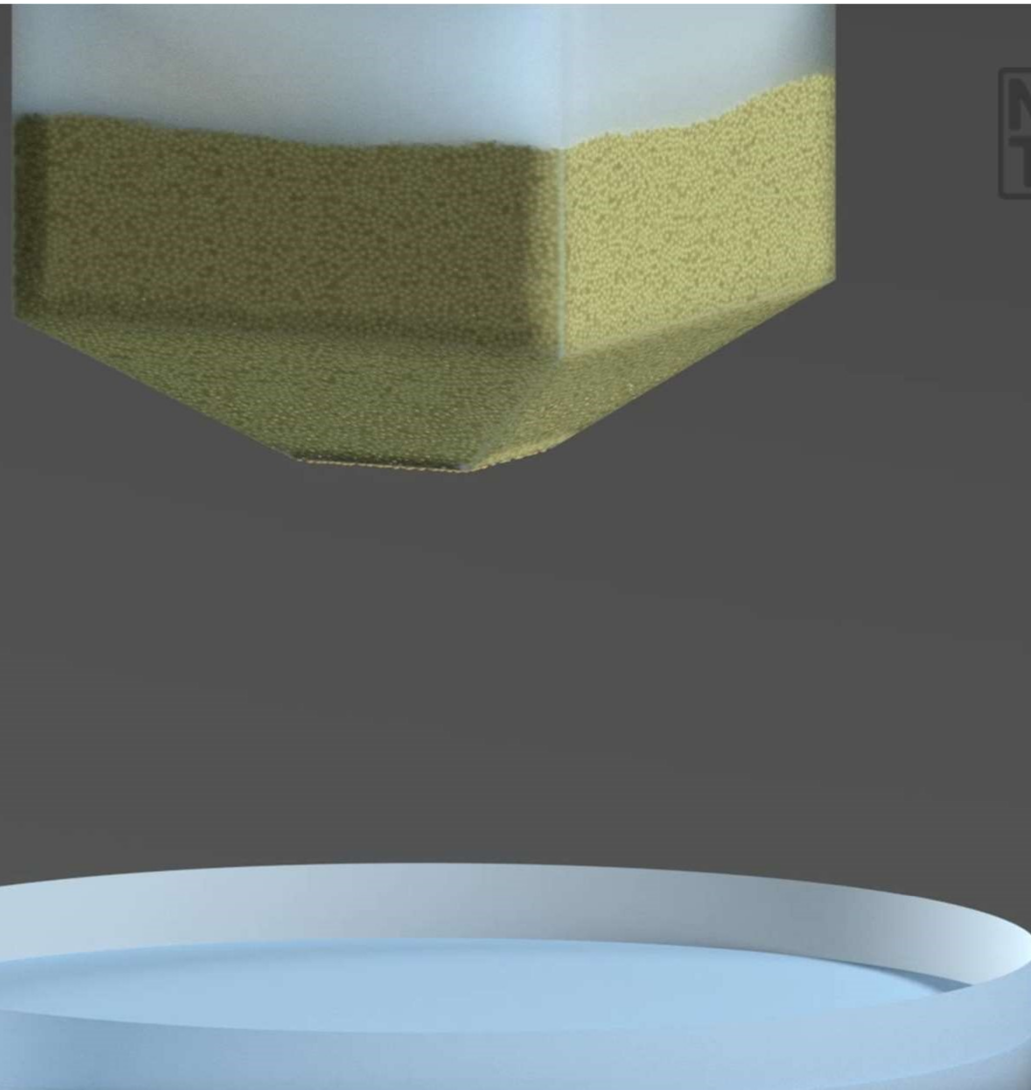
Powder dynamics meeting, October 10, 2017



Exascale simulation for the design of industrial-scale chemical reactors

M. Syamlal

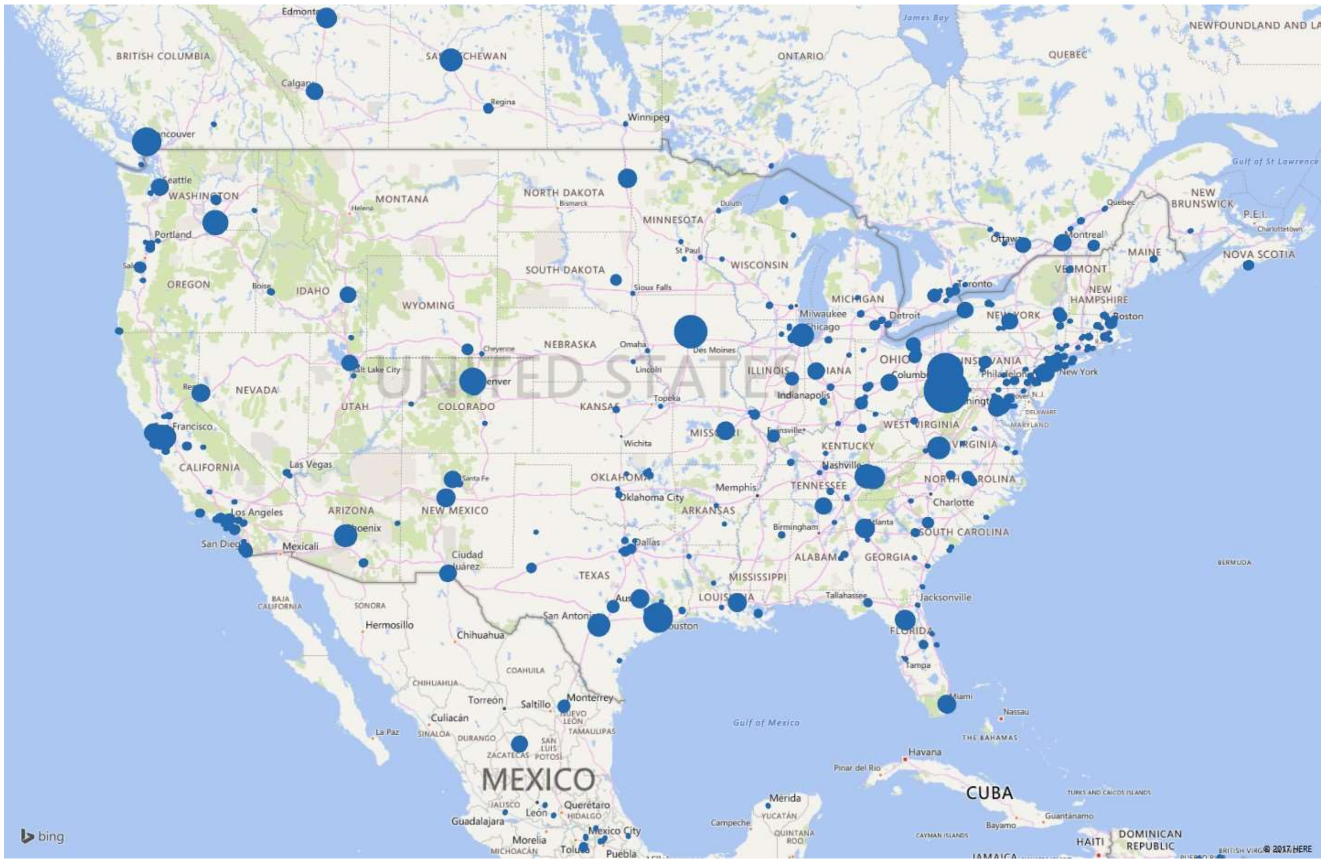
Senior Fellow

National Energy Technology Laboratory

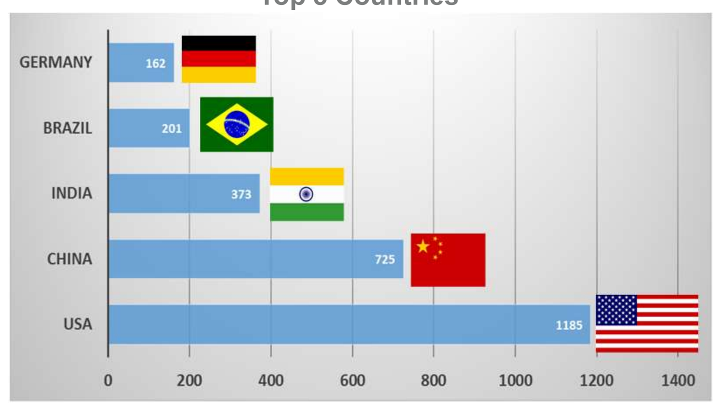
MFIX Overview

MFiX – Open-source multiphase CFD code

4,500+ all-time MFIX registrations

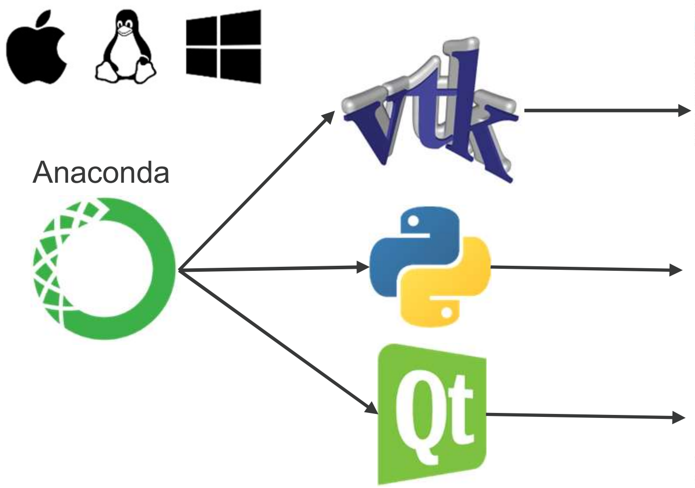


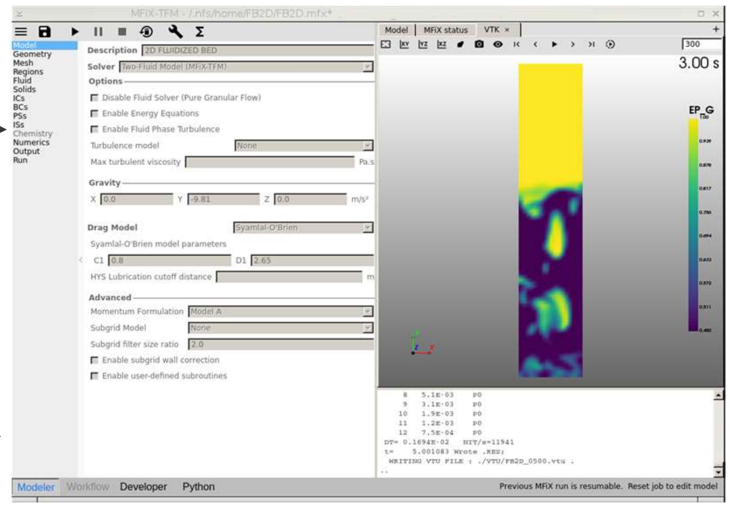
Top 5 Countries

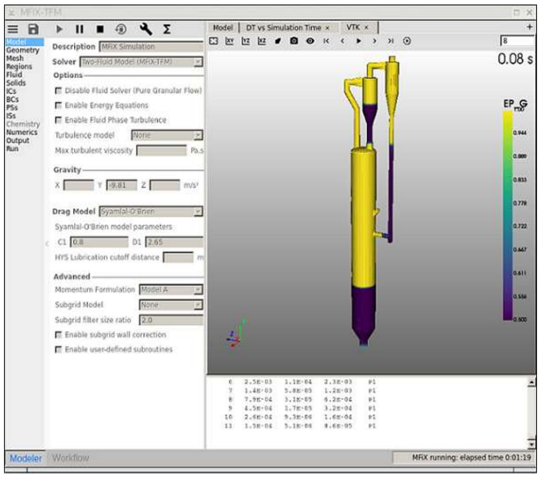


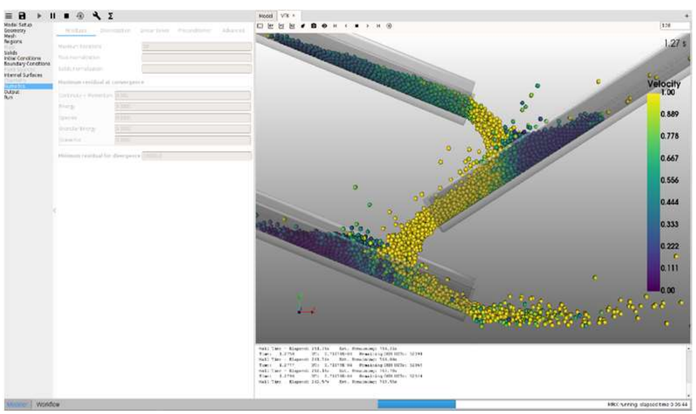
Examples of MFiX GUI

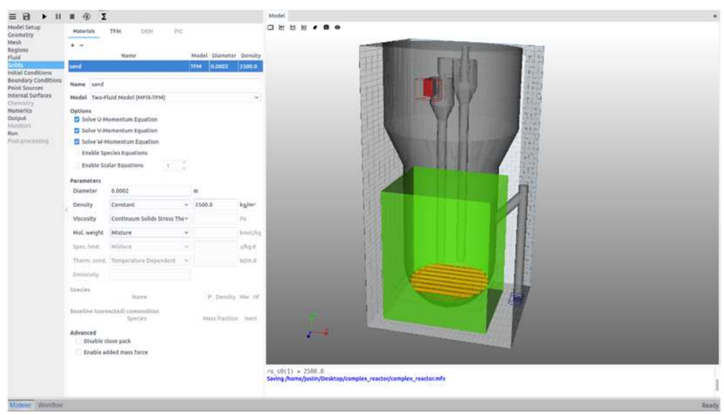
NATIONAL ENERGY TECHNOLOGY LABORATORY

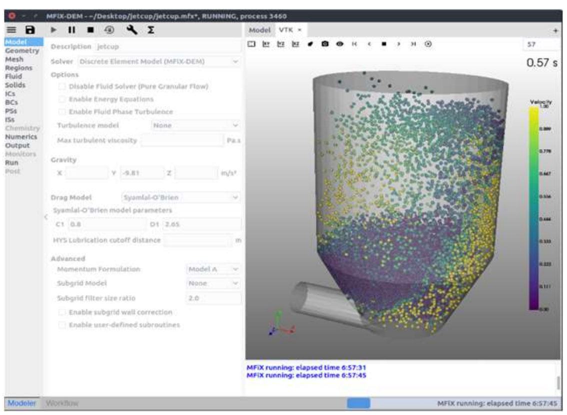




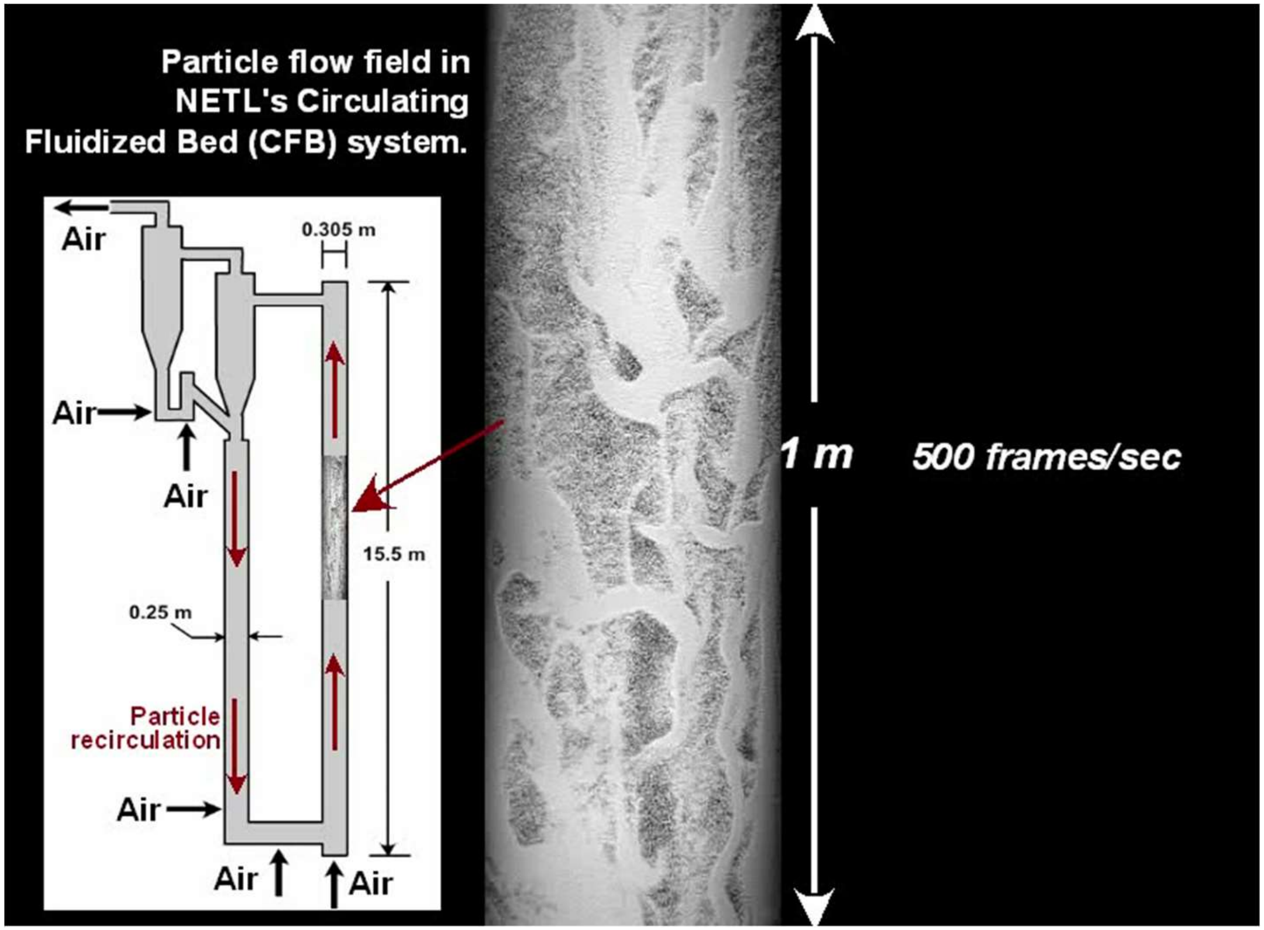








Gas-solids flow in a fluidized bed reactor



Shaffer F, Gopalan B. The Science and Beauty of Fluidization
arXiv:1311.1058v1 [physics.flu-dyn] 1 Nov 2013

MFiX offers a suite of multiphase models

NATIONAL ENERGY TECHNOLOGY LABORATORY

DNS ***Direct Numerical Simulation***: *Track all particles and resolve the gas flow around them*

MFiX DEM **Discrete Element Method**: Track all particles; use drag laws instead of resolving gas-solids boundary

MFiX Hybrid **Hybrid**: Some of the particle are tracked; others treated as a continuum

MFiX TFM **Two-Fluid Model**: Particles modeled as a continuum or a second fluid

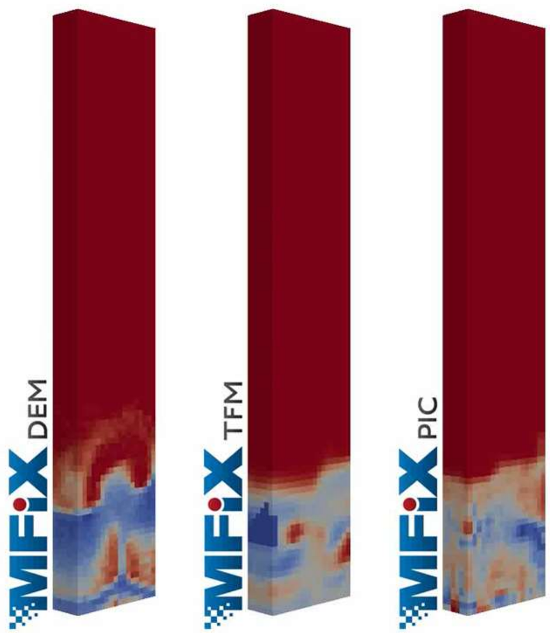
MFiX PIC **Particle-in-Cell** : Track parcels or clouds of particles

ROM ***Reduced Order Models***: *Simplified models for specialized applications*

Time to Solution

Development thrust

Model Uncertainty



CFD-DEM

Gas Phase – Navier-Stokes like equations

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \frac{\partial}{\partial x_j}(\varepsilon_g \rho_g U_{gj}) = 0$$

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g U_{gi}) + \frac{\partial}{\partial x_j}(\varepsilon_g \rho_g U_{gj} U_{gi}) = -\varepsilon_g \frac{\partial P_g}{\partial x_i} + \frac{\partial \tau_{gij}}{\partial x_j} + f_{gi} + \varepsilon_g \rho_g g_i$$

Particles – Newton's law

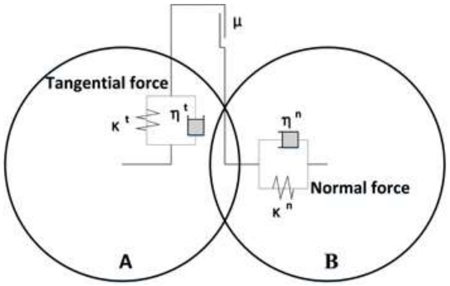
$$\frac{dx_{pi}}{dt} = u_{pi}$$

$$m_p \frac{du_{pi}}{dt} = m_p g_i + f_{pi} + m_p A_{coll}$$

$$I_{ij} \frac{d\omega_{pj}}{dt} = T_{pi}$$

- Unresolved flow near particle-fluid interface → gas-particle forces drag, added mass, lift …
- No numerical diffusion in particle phase
- Particle contacts are resolved

Soft-sphere model



A_{coll} describes both enduring contacts and collisions

MFiX DEM

Garg, R., Galvin, J., Li, T., and Pannala, S. (2012). Documentation of open-source MFIX–DEM software for gas-solids flows, From URL https://mfix.netl.doe.gov/documentation/dem_doc_2012-1.pdf

Two-Fluid Model

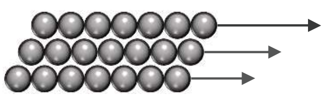
Gas and Granular Phases

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m) + \frac{\partial}{\partial x_j}(\varepsilon_m \rho_m U_{mj}) = 0$$

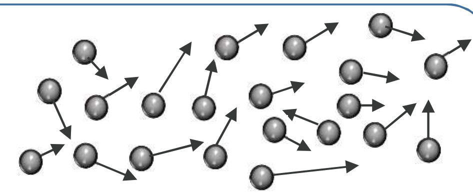
$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m U_{mi}) + \frac{\partial}{\partial x_j}(\varepsilon_m \rho_m U_{mj} U_{mi}) = -\varepsilon_m \frac{\partial P_g}{\partial x_i} + \frac{\partial \tau_{mij}}{\partial x_j} + \sum_{l=0}^{M} I_{mli} + \varepsilon_m \rho_m g_i$$

- Current workhorse in industry
- Cannot resolve distribution in particle-scale properties: size, density, chemical conversion
- Cannot describe regions where strain rate is zero
- Unresolved particle contacts → granular stress

Granular stress:



Frictional theory



Kinetic theory of granular flow

Granular energy transport equation

$$\frac{3}{2}\varepsilon_m \rho_m \left[\frac{\partial \Theta_m}{\partial t} + U_{mj}\frac{\partial \Theta_m}{\partial x_j}\right] = \frac{\partial}{\partial x_j}\left(\kappa_m \frac{\partial \Theta_m}{\partial x_j}\right) + \tau_{mvij}\frac{\partial U_{mi}}{\partial x_j} + \Pi_m - \varepsilon_m \rho_m J_m$$

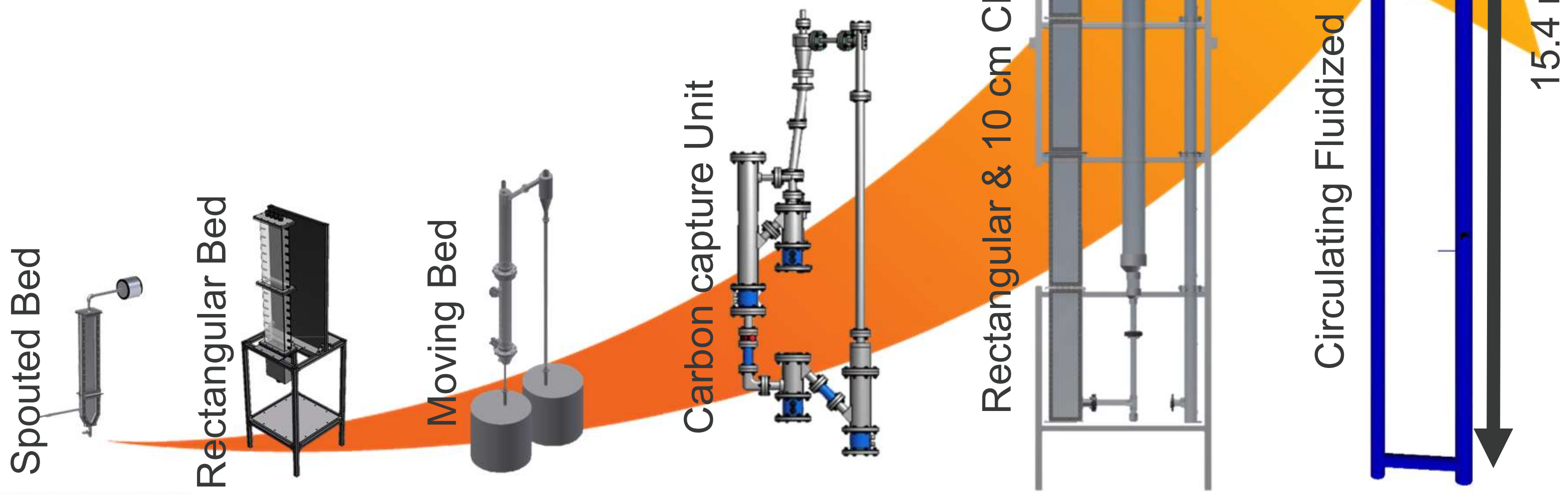
1. Syamlal, M., Rogers, W., & O'Brien, T. J. (1993). MFIX Documentation: Theory Guide (No. DOE/METC-94/1004 (DE94000087)
2. Benyahia, S., Syamlal, M., O'Brien, T.J., "Summary of MFIX Equations 2012-1", From URL https://mfix.netl.doe.gov/documentation/MFIXEquations2012-1.pdf , January 2012

Gas-solids flow research reactors

High-G Reactors

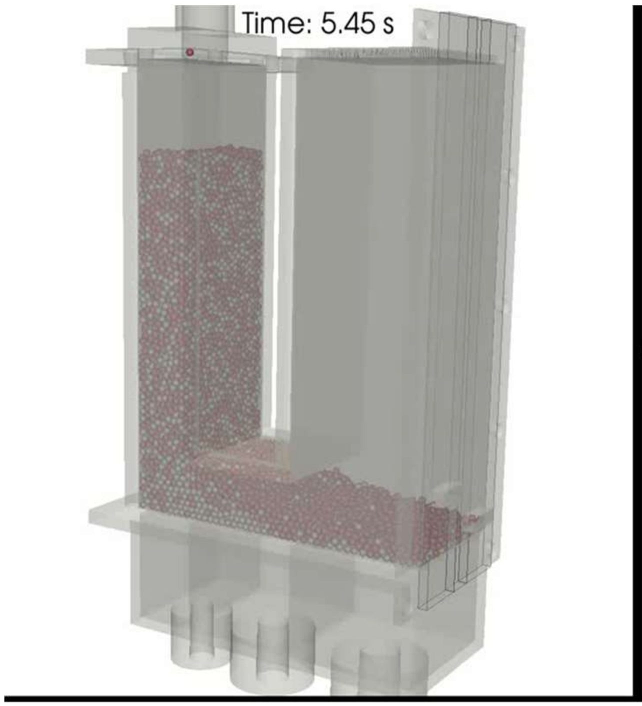
Rotating Fluidized Bed

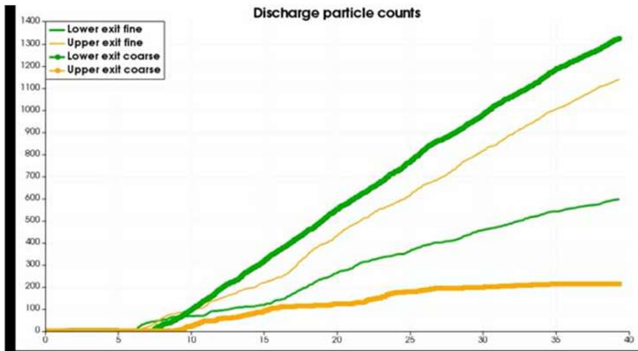
Vortex Bed

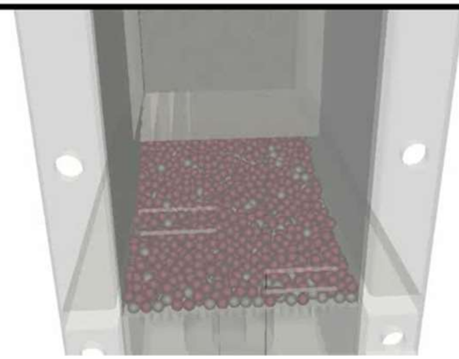


Reactor optimization based on CFD

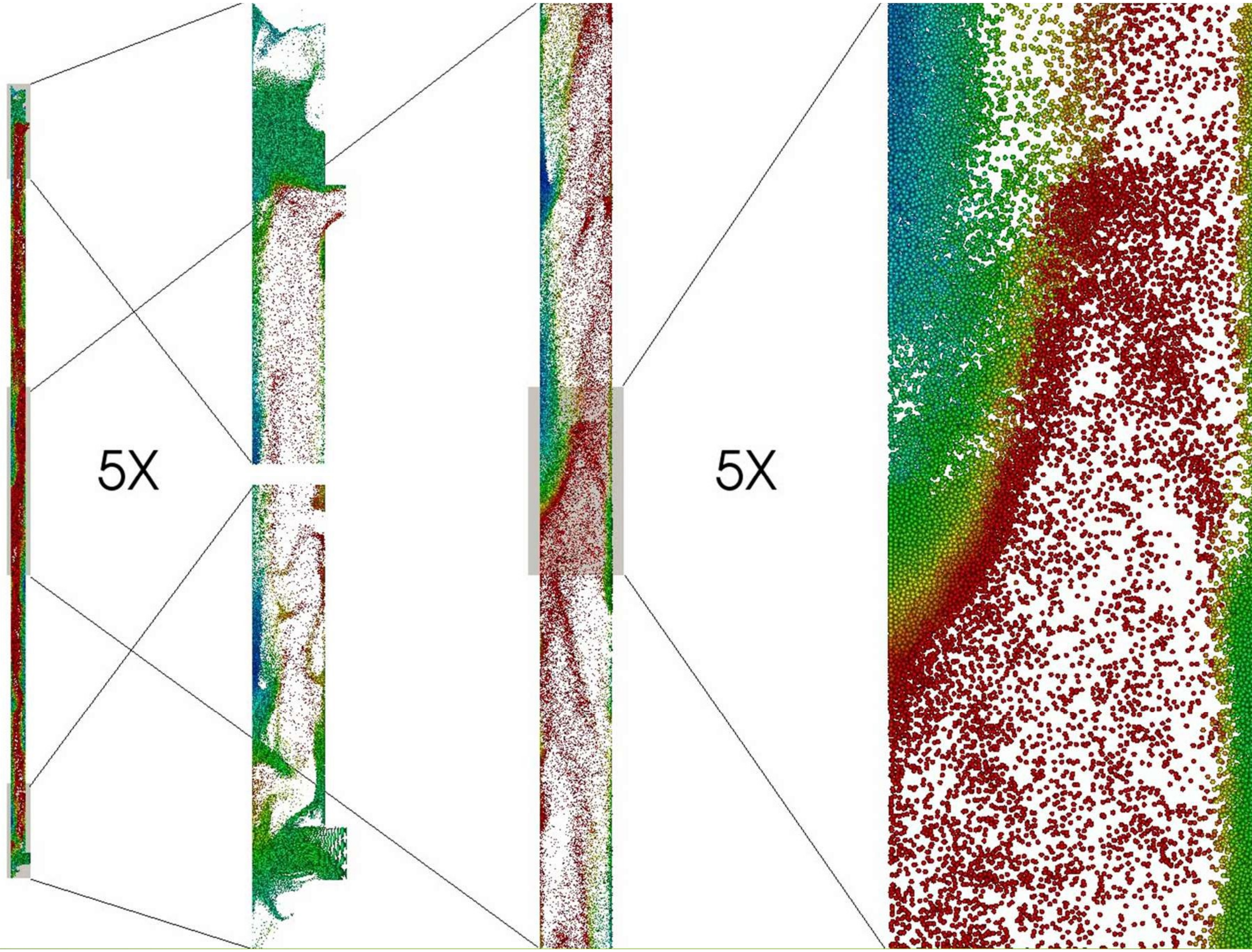
Optimized Flow for Separation – Model and Experiment



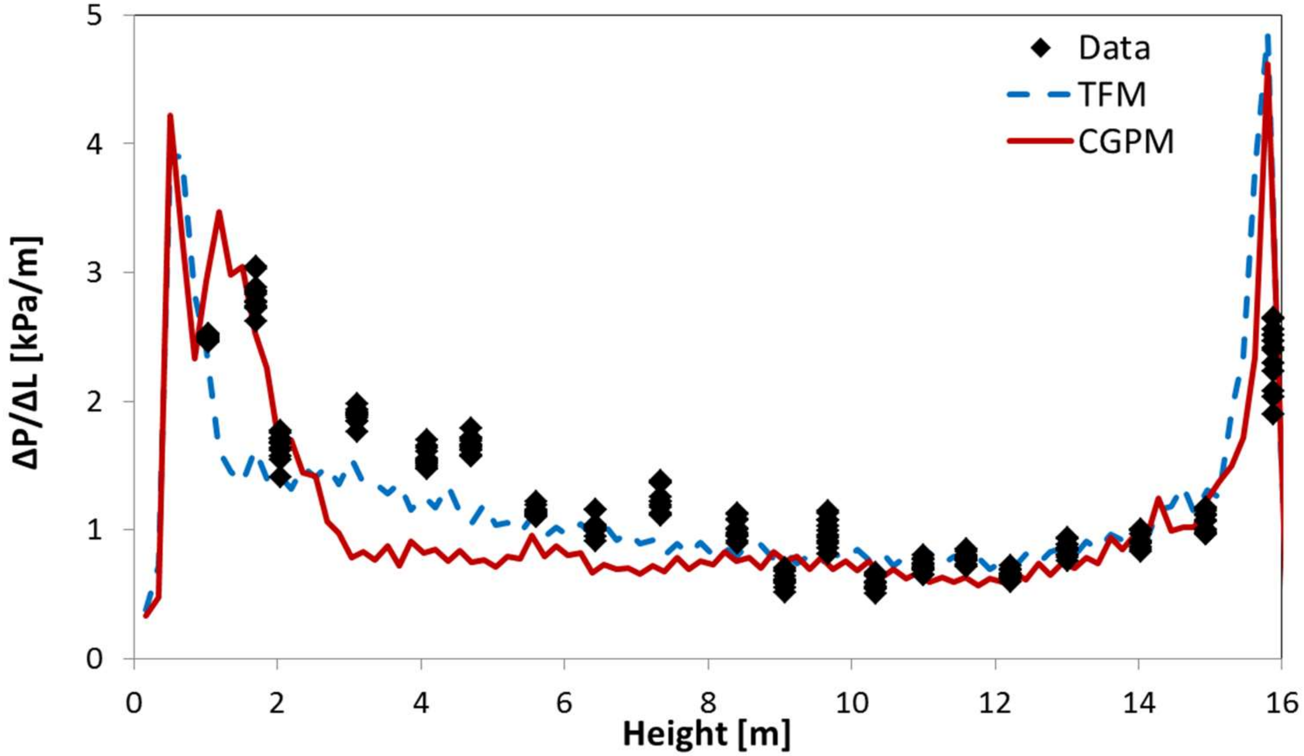




Mini circulating fluidized bed


5X
5X

Axial pressure gradient

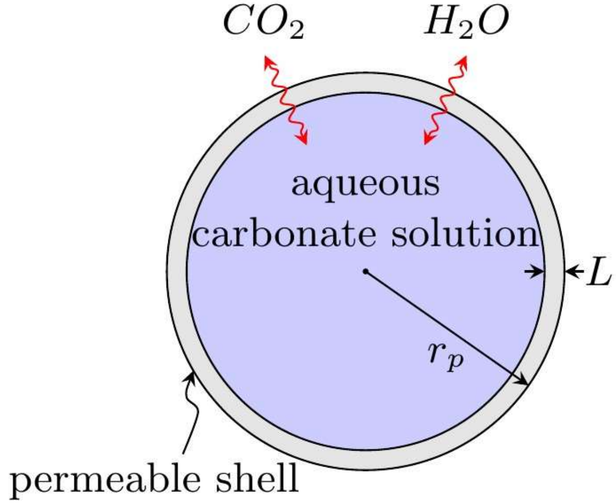


Comparison of MFIX-TFM and MFIX-DEM (Coarse-grained) results with experimental data

1. T. Li, MFiX simulations of gas-solid flow in large scale fluidized bed reactors, the 39th IFPRI Annual General Meeting, Jun. 17-21, 2017, Philadelphia.

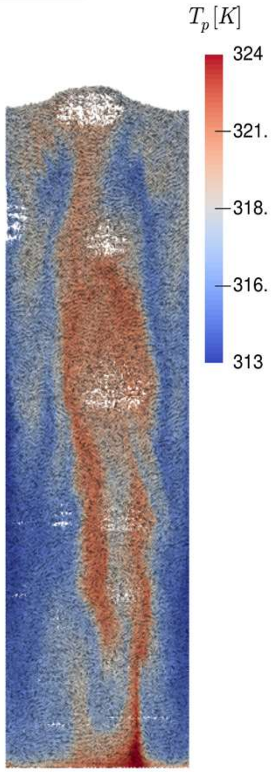
Micro-Encapsulated Carbon Sorbent (MECS)

MECS[1] capsules
(Image: John Vericella, LLNL)



- Elastic, deformable shell
- Capsule size/density changes
- Precipitation of solids inside capsule
- Water loss/uptake during CO_2 capture
- Complex liquid equilibrium reactions

MECS Capsule model

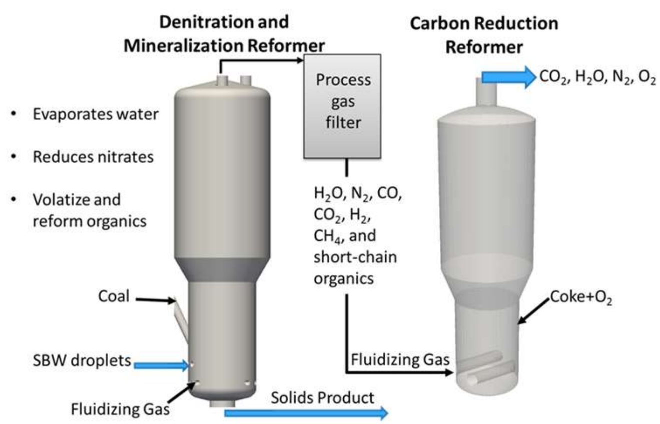


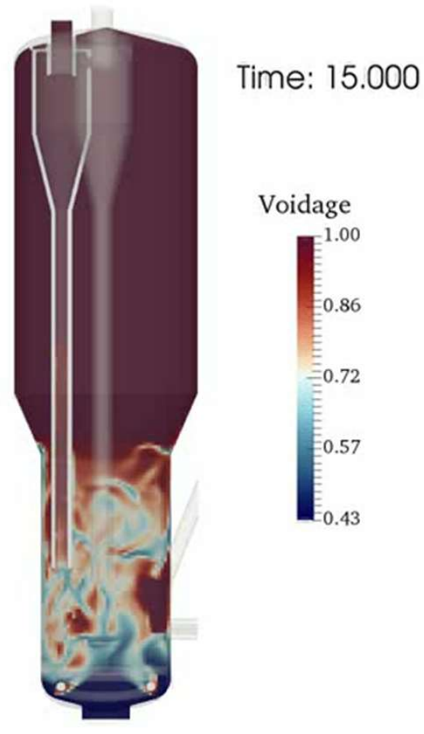
MECS fluidized bed simulation

[1]Vericella et al., *Nature Comms.*, v. 6, 2015

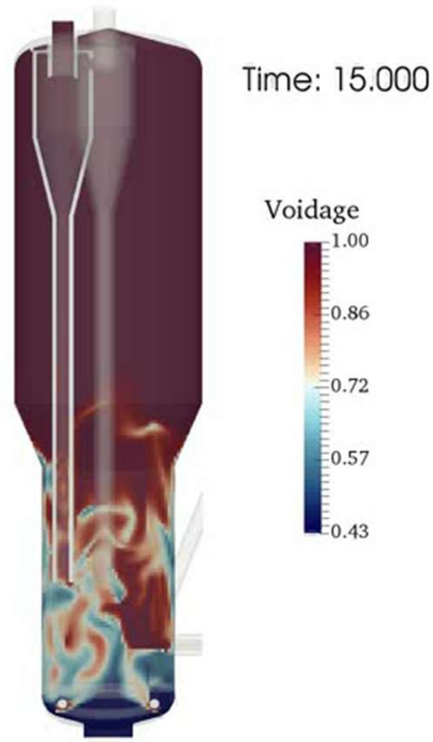
Integrated Waste Treatment Unit, Idaho

Guide performance improvement of nuclear waste clean up reactor

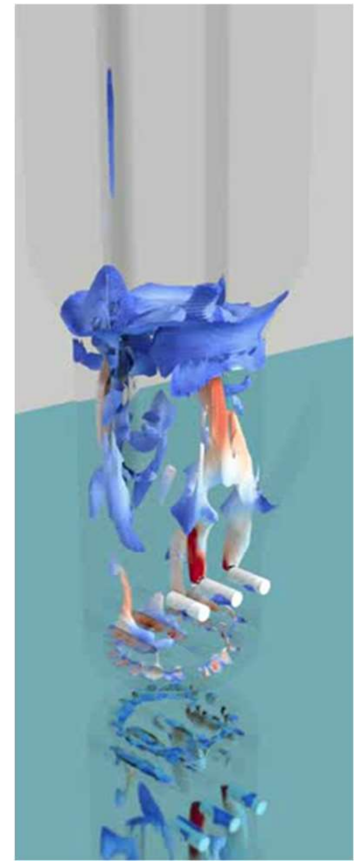




Low Flow
0.6 gpm

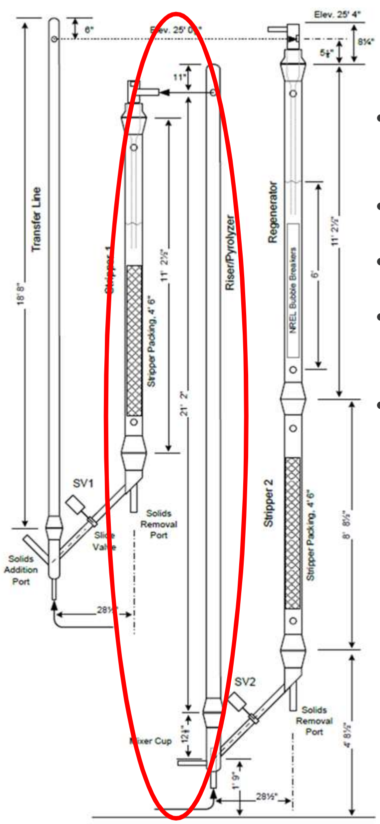


High Flow
1.25 gpm



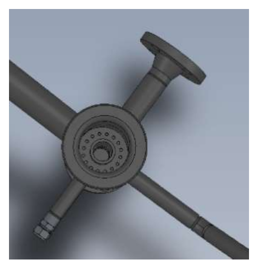
Biofuels reactor

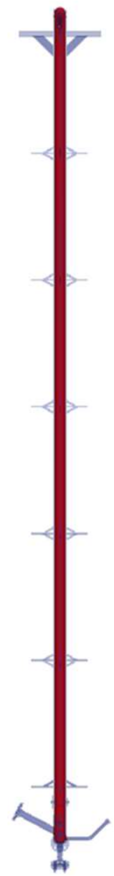
Upgrading reactor models to help pilot-scale testing



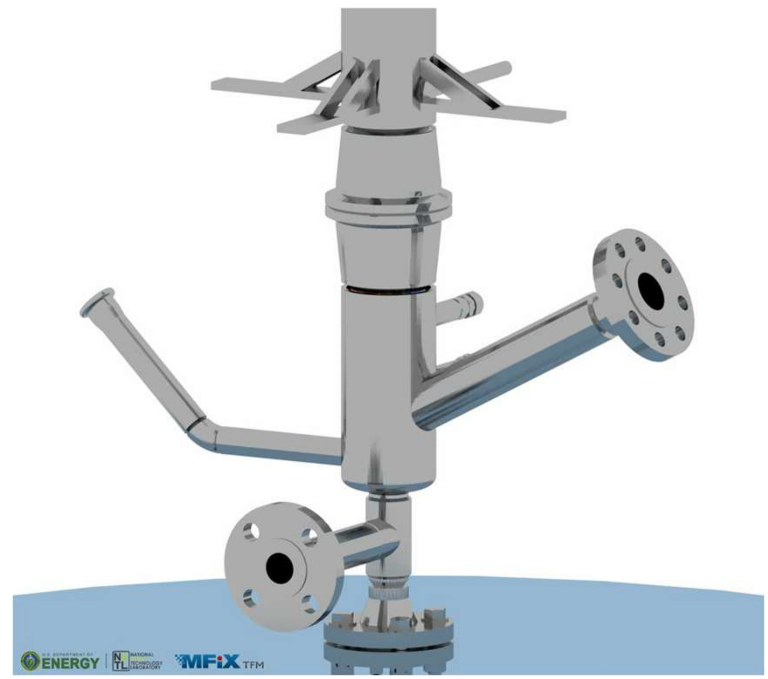
Upgrading Reactor

- Riser: Height: 7.05 m, diameter: 0.092 m
- Outlet diameter: 0.038 m
- Solids inlet diameter: 0.049 m
- Pyrolysis vapor inlet diameter: 0.047 m
- Distributor: 16 holes with diameter of 0.00625 m





Riser Geometry



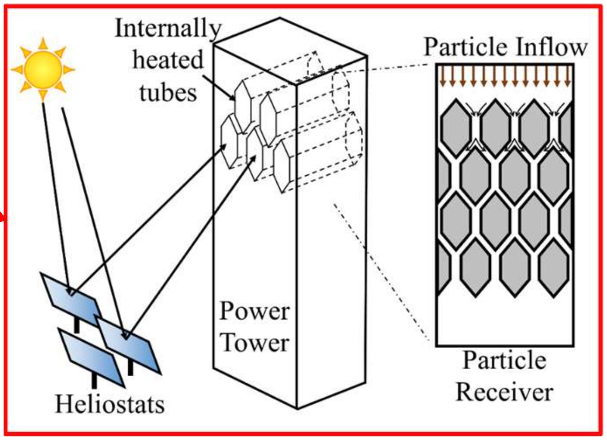
Using Solids as Heat Transfer "Fluid" for CSP Receivers

Challenge: Molten salts unstable > 600∘C

Idea: Use inert solids (e.g., sand) as heat transfer "fluid"

- can operate at higher T and thus increased efficiency
- good thermal storage for on/off diurnal cycle
- Sand is inexpensive

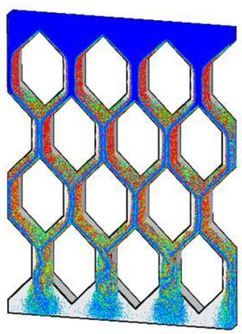
CSP Power Tower



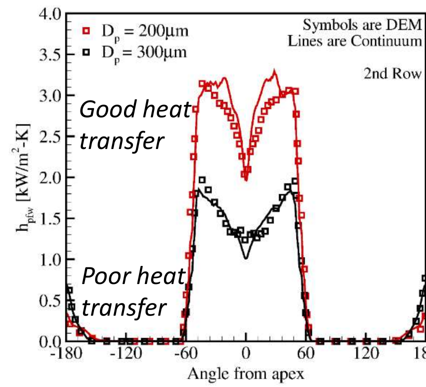
PI: Christine Hrenya (Univ. CO)
Co-PI's: Zhiwen Ma (NREL)
Sreekanth Pannala (ORNL)

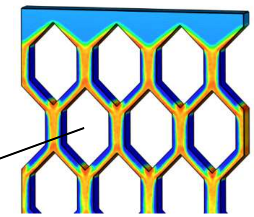
Using Solids as Heat Transfer "Fluid" for CSP Receivers

MFIX DEM simulations
(~10^7 particles on Titan)

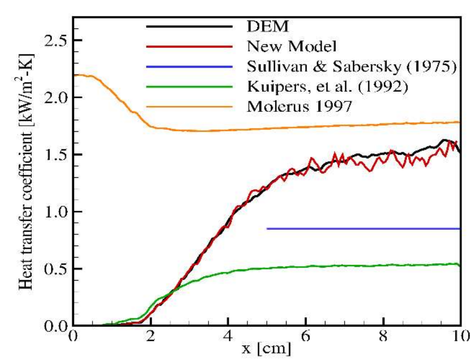


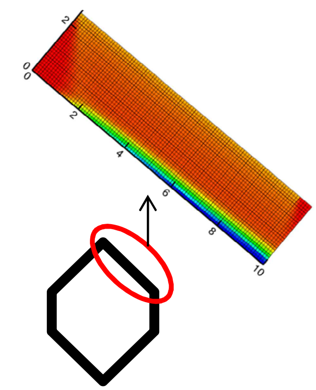
Informed design





Drove development of continuum theory





Morris et al., *AIChE J.* (2016)
Morris et al., *Solar Energy* (2016)
Morris et al., *Int. J. Heat Mass Transfer* (2015)

Colorado NREL NATIONAL RENEWABLE ENERGY LABORATORY OAK RIDGE National Laboratory SunShot U.S. Department of Energy

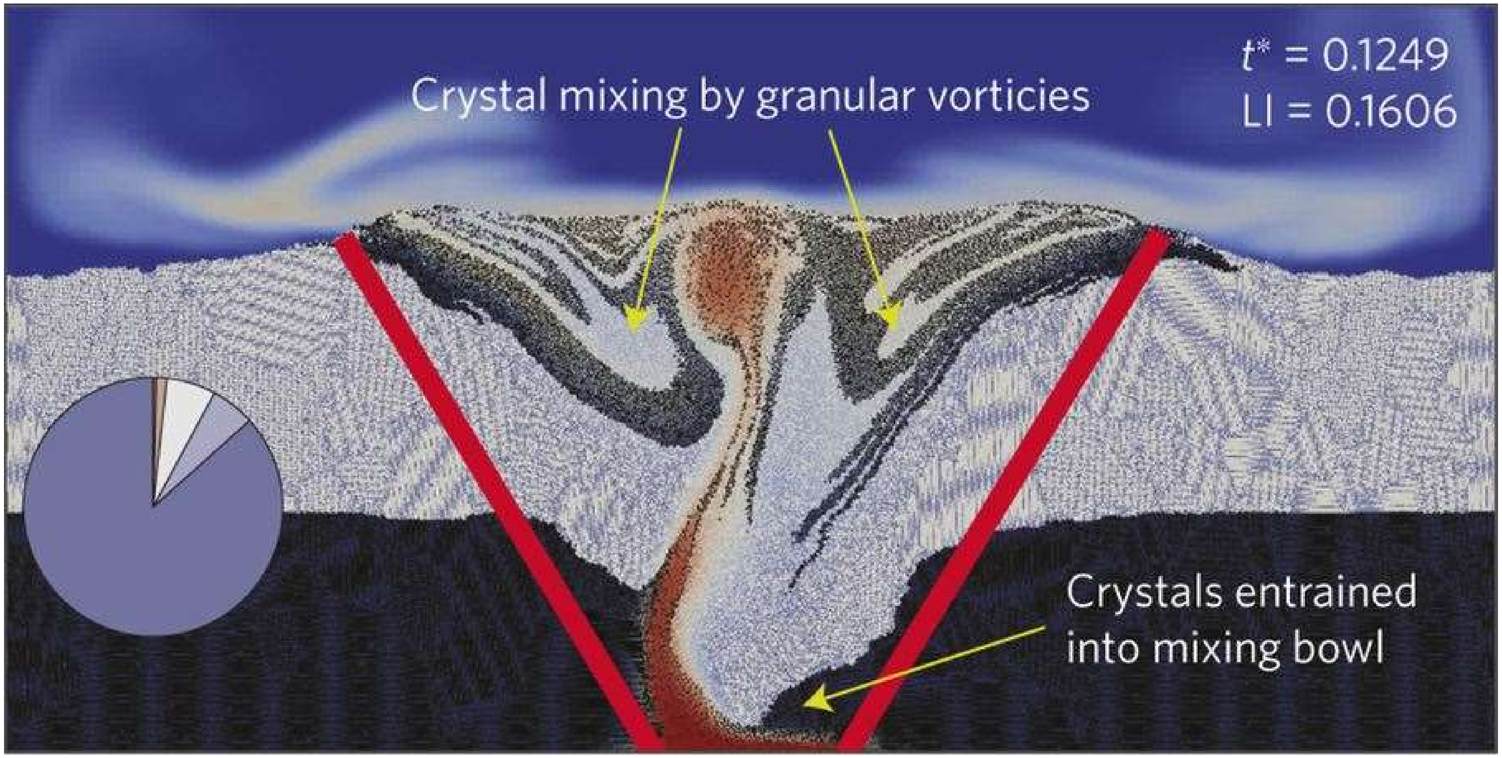
Volcanic hazards from explosive eruptions

Soufrière Hills volcano   MFiX-TFM simulation

1. Dufek, J., and Bergantz, G.W, 2007, “Dynamics and deposits generated by Kos Plateau Tuff eruption”, G3, vol. 8, no. 12
2. Ruprecht, P., Bergantz, G.W. and Dufek, J., 2008, “Modeling of gas driven magmatic overturn”, G3, vol. 9, no. 7.
3. Dufek, J. and Manga, M., 2008, “In situ production of ash in pyroclastic flows”, J. Geophysical Res., vol. 113

George Bergantz/University of Washington

Path of ‘magma mush’ inside a volcano



G.W. Bergantz, J. M. Schleicher and A. Burgisser, 2015. “Open-system dynamics and mixing in magma mushes”, Nature Geoscience, 8, 793-797.

George Bergantz/University of Washington

MFiX DEM

MFIX-Exa Project

Acknowledgments

This research was supported by the Exascale Computing Project (http://www.exascaleproject.org), a joint project of the U.S. Department of Energy's Office of Science and National Nuclear Security Administration, responsible for delivering a capable exascale ecosystem, including software, applications, and hardware technology, to support the nation's exascale computing imperative.

Project Number: 1.2.1.21

EXASCALE COMPUTING PROJECT

National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY | Office of Science

www.ExascaleProject.org

The Exascale Computing Project (ECP)

Collaboration

2 US Department of Energy organizations

- Office of Science
- National Nuclear Security Administration

Execution

800 researchers (22 laboratory and agency partners; 39 universities) engaged in:

- 66 software projects
- 25 science application projects
- 5 co-design centers

Goal

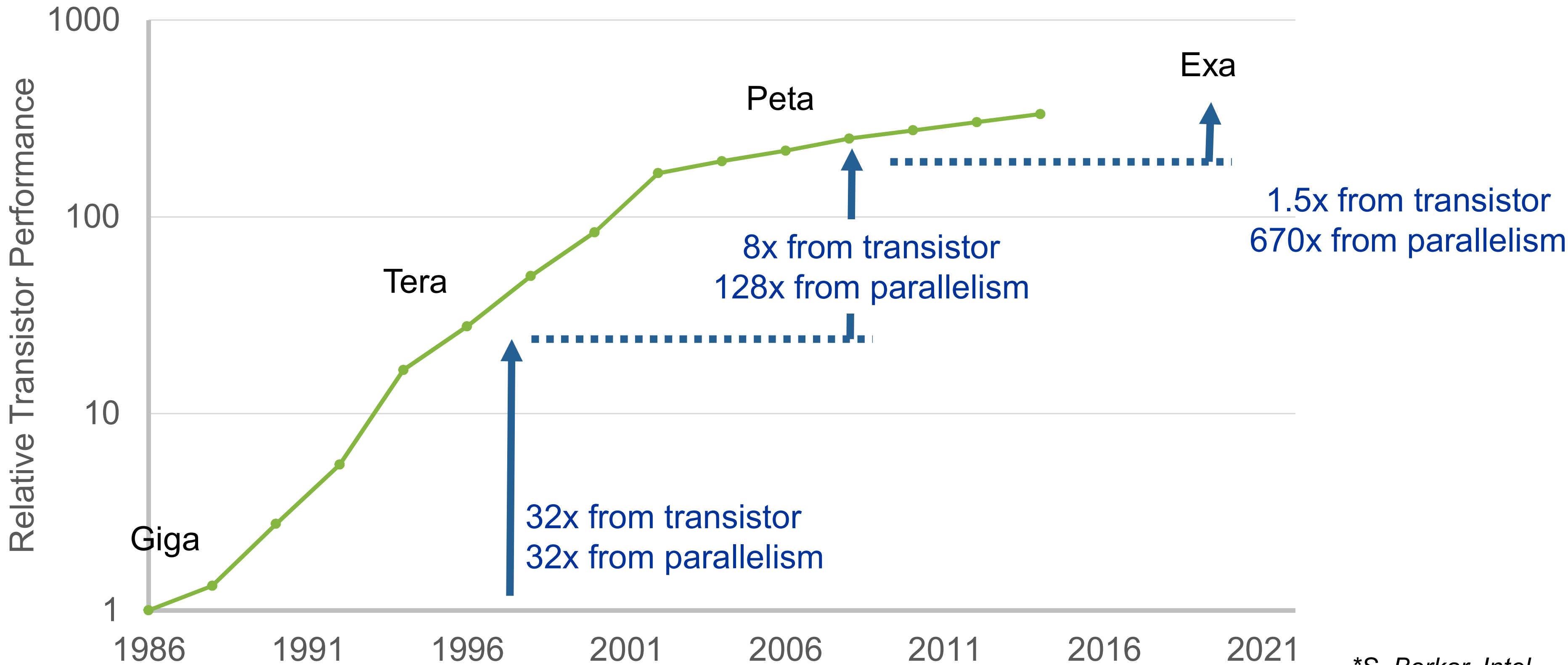
Drive pre-exascale science, application development, hardware and software R&D to ensure that the US has a **capable exascale ecosystem** in 2021

What is a capable exascale computing system?

- Delivers 50× the performance of today's 20 PF systems, supporting applications that deliver high-fidelity solutions in less time and address problems of greater complexity
- Operates in a power envelope of 20–30 MW
- Is sufficiently resilient (perceived fault rate: ≤1/week)
- Includes a software stack that supports a broad spectrum of applications and workloads

This ecosystem will be developed using a co-design approach to deliver new software, applications, platforms, and computational science capabilities at heretofore unseen scale

From Giga to Exa, via Tera & Peta*



*S. Borkar, Intel

Performance from parallelism

Exascale simulation for the design of industrial-scale chemical reactors

Goal: Develop an efficient high-fidelity multiphase flow modeling capability to aid in the design of industrial-scale chemical reactors

Simulation with high-fidelity, physics-based models is essential to scaling up from lab → pilot → commercial scale reactors

- Reduction in cost
- Reduction in time to deployment
- Risk mitigation at large scales

Proposed increase in fidelity will aid in the development of CO_2 capture technology (supported by DOE-FE) as well as unlock the ability to simulate a host of relevant problems in energy, chemical processing and pharmaceutical industries

Lab-scale testing of a novel CO_2 capture method at NETL

Petra Nova, world's largest post-combustion CO_2 capture plant, began operation in January 2017

MFIX-Exa challenge problem

Simulate 1 MWe chemical looping reactor with CFD-DEM

2017

Particle Count: 60 x10^6

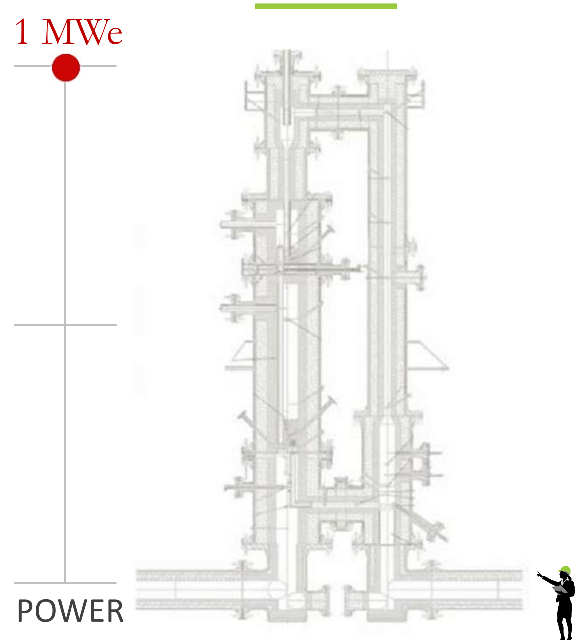
Time to Solution: 600 days

2023

Particle Count: 5 x10^9

Time to Solution: 0.5 days

2026



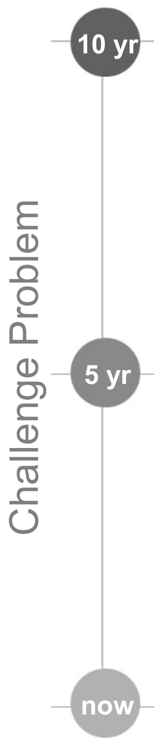
Particle Count: 100 x 10^9

Time to Solution: 2 days

Time-to-solution is estimated for 5 minutes of real time in all cases; the 2023/2026 values are guestimates.

Achieving the desired performance in MFIX-Exa

The 10 Year Challenge Problem

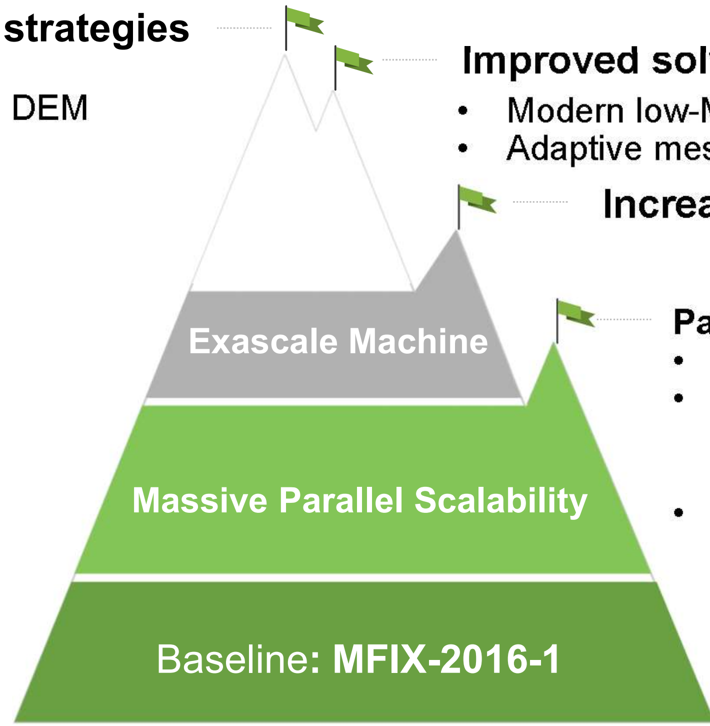


Risk mitigation strategies
- Hybrid method
- Coarse grained DEM

Improved solver
- Modern low-Ma projection method
- Adaptive mesh refinement

Increased computational power

Parallel Performance
- Balanced fluid & particle work load
- Optimized particle-particle interaction tracking: increased on-node performance and reduced off-node communication
- Scalable linear equation solver



MFIX-Exa brings together three teams and two codes

NATIONAL ENERGY TECHNOLOGY LABORATORY | BERKELEY LAB | Boulder

- 60+ years of experience in multiphase modeling and MFIX (NETL and CU)
- 60+ years of experience in large-scale, multiscale multiphysics applications (LBNL)
- 90+ years of experience in high performance computing

MFiX Exa

MFiX + AMReX

MFiX

- 30+ years of development
- 12 developers at NETL
- 4,000+ registered users
- 175+ downloads per month
- 200+ citations per year
- Applied for reactor design and troubleshooting in fossil, bio, nuclear, and solar energy; chemicals industry; and nuclear waste treatment

AMReX

- Block-structured AMR software framework supported by ECP Co-Design Center
- Supports multiple DOE codes: accelerator modeling, astrophysics, combustion, cosmology, and subsurface
- Long development history

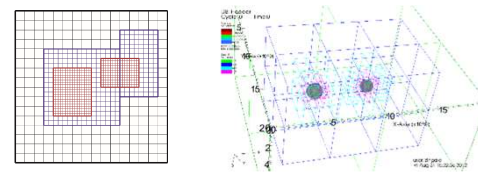
AMReX

Block-Structured Adaptive Mesh Refinement Framework. Support for hierarchical mesh and particle data with embedded boundary capability.

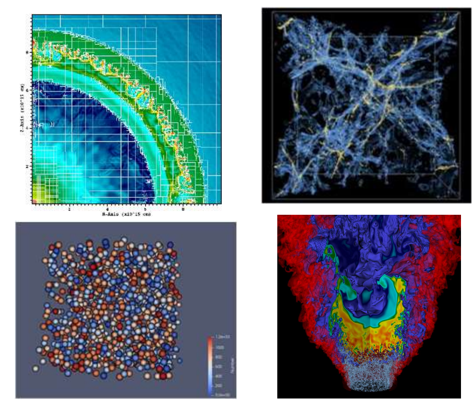
Open source software

- Support for solution of PDE's on hierarchical adaptive mesh with particles and embedded boundary representation of complex geometry
  - Core functionality in C++ with frequent use of Fortran90 kernels
- Support for multiple modes of time integration
- Provides support for explicit and implicit single-level and multilevel mesh operations, multilevel synchronization, particle, particle-mesh and particle-particle operations
- Hierarchical parallelism -- hybrid MPI + OpenMP with logical tiling to work efficiently on new multicore architectures
- Native multilevel geometric multigrid solvers for cell-centered and nodal data
- Highly efficient parallel I/O for checkpoint/restart and for visualization – native format supported by Visit, Paraview, yt

https://www.github.com/AMReX-Codes/amrex



Examples of 2D and 3D grids

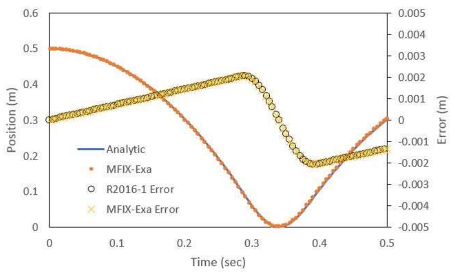


Examples of AMReX applications

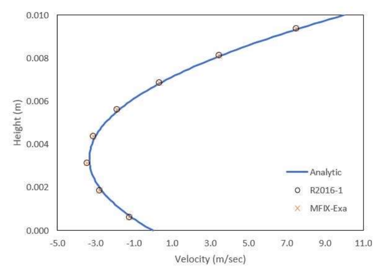
Applications: accelerator modeling, astrophysics, combustion, cosmology, multiphase flow…

First version of MFIX-Exa developed and verified

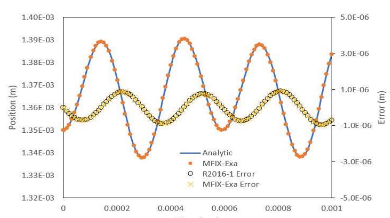
Many verification cases



Freely falling particle with wall collision

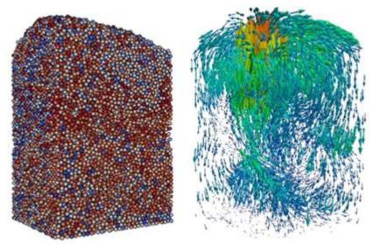


Couette flow in a channel

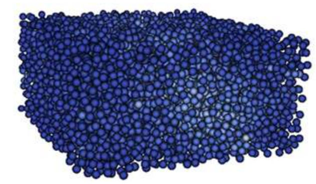


Two stacked compressed particles

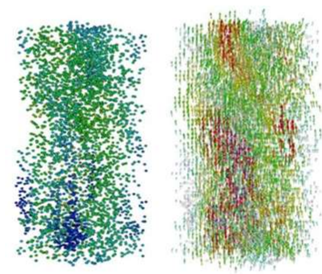
Four benchmark cases that mimic sections of a CLR



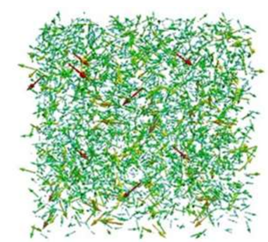
Fluidized Bed



Settling Bed

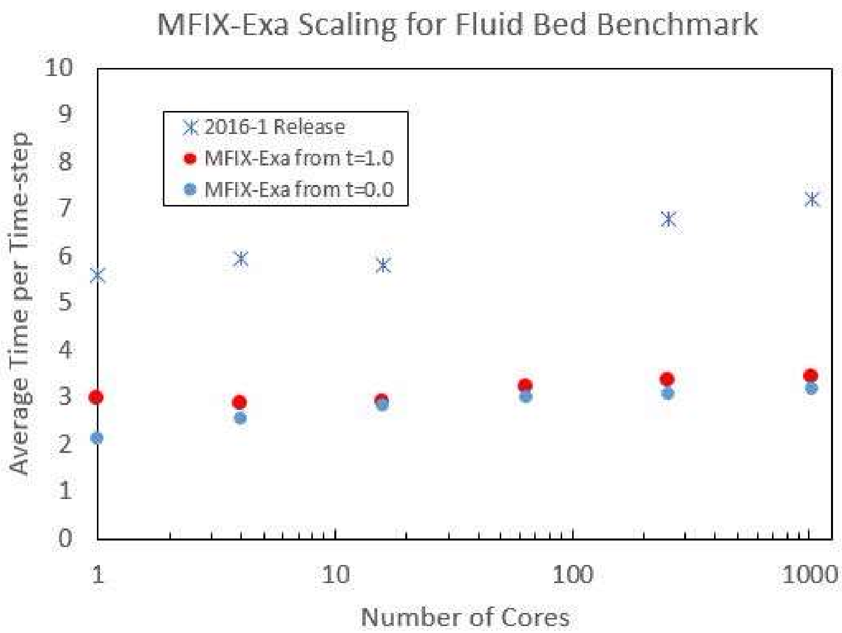


Riser Flow



Homogeneous Cooling System

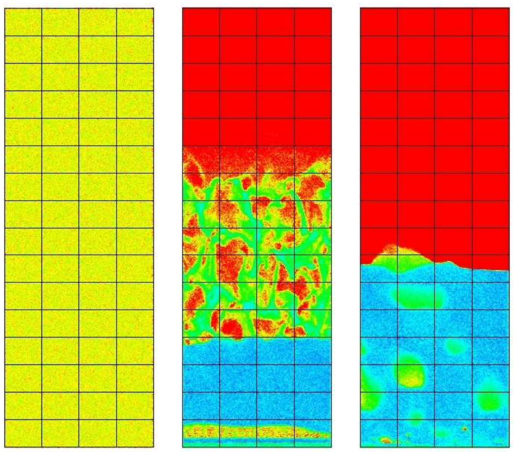
Preliminary performance analysis conducted



Scaling of MFIX-Exa and MFIX-2016-1 Release on Cori-KNL (run for 50ms)

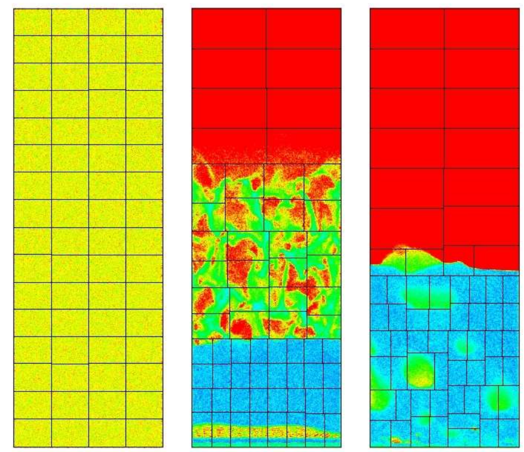
MFIX-Exa released with hybrid parallelism and dynamic load balancing

- Take full advantage of many-core architectures through Hybrid parallelism (MPI + OpenMP)
- Minimize run time through Dynamic load balancing



Based on number of grid cells

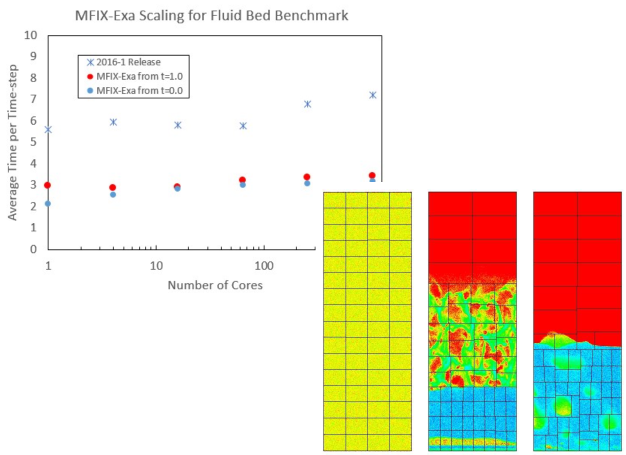
Two load balancing strategies



Based on number of particles

MFIX-Exa Status and Development Plans

Migrated MFIX-DEM hydrodynamics to the AMReX framework.



EB Particles

Replace SIMPLE

EB Fluid

Performance!
Performance!
Performance!

CLR Demonstration

2017

2018

2019

NATIONAL ENERGY TECHNOLOGY LABORATORY

BERKELEY LAB

Boulder

MFiX Exa

ECP EXASCALE COMPUTING PROJECT

Thank You!

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